May 8, 2003

Sarah Loftus McLallen
Manager, CHEMSTAR
The American Chemistry Council Petroleum Additives
Panel Health, Environmental and Regulatory Task Group
1300 Wilson Boulevard
Arlington, VA 22209

Dear Ms. McLallen:

The Office of Pollution Prevention and Toxics is transmitting EPA's comments on the robust summaries and test plan for Arylpolyolefins posted on the ChemRTK HPV Challenge Program Web site on January 15, 2003. I commend The American Chemistry Council's Petroleum Additives Panel Health, Environmental and Regulatory Task Group for their commitment to the HPV Challenge Program.

EPA reviews test plans and robust summaries to determine whether the reported data and test plans will provide the data necessary to adequately characterize each SIDS endpoint. On its Challenge Web site, EPA has provided guidance for determining the adequacy of data and preparing test plans used to prioritize chemicals for further work.

EPA will post this letter and the enclosed comments on the HPV Challenge Web site within the next few days. As noted in the comments, we ask that The American Chemistry Council's Petroleum Additives Panel Health, Environmental and Regulatory Task Group advise the Agency, within 60 days of this posting on the Web site, of any modifications to its submission.

If you have any questions about this response, please contact Richard Hefter, Chief of the HPV Chemicals Branch, at 202-564-7649. Submit questions about the HPV Challenge Program through the "Contact Us" link on the HPV Challenge Program Web site pages or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsca-hotline@epa.gov.

I thank you for your submission and look forward to your continued participation in the HPV Challenge Program.

Sincerely,

-S-

Oscar Hernandez, Director
Risk Assessment Division

Enclosure

cc: C. Auer
A. Abramson
W. Penberthy
M. E. Weber

EPA Comments on Chemical RTK HPV Challenge Submission:
Arylpolyolefins Category

Summary of EPA Comments

The sponsor, the American Chemistry Council Petroleum Additives Panel, submitted a test plan and robust summaries to EPA for the arylpolyolefins category dated December 18, 2002. EPA posted the submission on the ChemRTK HPV Challenge Web site on January 15, 2003. The category consists of C_{14}-C_{24} branched and linear alkyl derivatives of benzene (CAS No. 115733-08-9) and polypropylene derivatives of benzene (CAS No. 68081-77-6).

EPA has reviewed this submission and has reached the following conclusions:

1. Category Justification. Grouping the two chemicals on the basis of structural similarity and physicochemical properties is reasonable for health and ecological effects.

2. Physicochemical Properties. The submitted data for boiling point, vapor pressure, and partition coefficient are adequate for the purposes of the HPV Challenge Program. EPA agrees with the submitter's plan to test for water solubility. In addition, the submitter needs to provide a discussion on melting point in robust summary format.

3. Environmental Fate. The submitted data for photodegradation and stability in water are adequate for the purposes of the HPV Challenge Program. For transport and distribution, EPA recommends the use of EQC level III. EPA does not agree with the submitter's proposed biodegradation testing for only the C14-C24 alkaryl derivative. The submitter needs to test both chemicals because the wide range of molecular weights and differing branching structures may result in differing biodegradation results for the two category members.

4. Health Effects. EPA agrees with the submitter's plan to conduct chromosomal aberrations and combined repeated-dose/reproduction/developmental toxicity screening tests.

5. Ecological Effects. No aquatic toxicity data are available to characterize category members. However, EPA recommends no acute or chronic testing because estimated water solubility and log Kow values suggest that no toxicity is expected to occur.

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.

EPA Comments on the Arylpolyolefins Category Challenge Submission

Category Definition

The category includes two long-chain alkyl derivatives of benzene: C_{14}-C_{24} branched and linear alkyl derivatives (CAS No. 115733-08-9) and polypropylene derivatives (CAS No. 68081-77-6). The substance, C_{14}-C_{24} branched and linear alkyl derivatives of benzene has a carbon number range for the alkyl side chain of C_{14}-C_{24}, and a corresponding molecular weight range of 275 to 415. The total carbon number range for the commercially available form of polypropylene derivatives is C_{22}-C_{82} (information available only in the robust summary) and the corresponding molecular weight range is 387 to 1228. The category definition is adequate.

Category Justification

The submitter bases the arylpolyolefin category on structural similarity, the similarity of estimated physicochemical properties and similar stabilities in water, rates of photodegradation, and acute mammalian toxicity.

Although there are some differences in vapor pressure, water solubility, and log Kow values, the submitter has provided sufficient evidence to show that the C_{14}-C_{24} alkaryl derivatives and polypolefin derivatives will partition similarly in the environment, undergo similar rates of photodegradation, and will not be susceptible to hydrolysis.

Toxicological support for the category is limited to acute mammalian toxicity data. In acute oral and dermal toxicity tests, neither compound caused lethality at the limit dose of 5000 mg/kg.

Although no data were available for the acute fish, invertebrate, and algal toxicity endpoints of the arylpolyolefins, their high log K_{ow} (greater than 8) and low water solubility values suggest negligible toxicity.

Overall, the available information supports the category with the exception of biodegradation; the C_{14}-C_{24} alkaryl derivative side chains are mostly linear and are anticipated to degrade more readily than the branched side chains of the polypropylene derivatives. These differences are likely to be significant and are not accounted for in the test plan.

Test Plan

Physicochemical Properties (melting point, boiling point, vapor pressure, partition coefficient and water solubility).

The submitted data for boiling point, vapor pressure, and partition coefficient are adequate for the purposes of the HPV Challenge Program. EPA found measured data on similar substances that are consistent with the estimated values for the sponsored chemicals. EPA agrees with the submitter's approach to water solubility.

Melting Point. In addition to the test plan, the submitter needs to include the melting point discussion in robust summary format.

Environmental Fate (photodegradation, stability in water, biodegradation, fugacity).

The submitted data for photodegradation and stability in water are adequate for the purposes of the HPV Challenge Program.

Biodegradation. EPA disagrees with the submitter's plan to test the biodegradation of the C_{14}-C_{24} alkaryl derivative and read across to the polypropylene derivative. The submitter expects the C_{14}-C_{24} alkaryl derivative to biodegrade to a high extent and the polypropylene derivative to have a limited potential to biodegrade. EPA believes the wide range of molecular weights and differing branching structures may result in differing biodegradation results for the two category members and thus testing only the one substance will provide only an upper limit for biodegradation for the category. Therefore, EPA believes that the use of a read across approach for biodegradation is not appropriate in this case and recommends that the submitter needs to provide ready biodegradation data for both chemicals following OECD TG 301.

Fugacity. The sponsor estimated the fugacity of these chemicals using a Level I EQC model. Although EPA had previously recommended the use of EQC Level I, this model is somewhat limited. EPA now recommends the use of the EQC level III model, which provides a more rigorous level of analysis. EPA

believes that values based on a level III fugacity model are more realistic and useful for estimating a chemical's fate in the environment on a regional basis.

Health Effects (acute toxicity, repeated-dose toxicity, genetic toxicity, and reproductive/developmental toxicity).

Adequate data are available for acute toxicity and gene mutations endpoints for the purposes of the HPV Challenge Program.

The submitter is proposing to conduct an in vitro chromosomal aberrations test and a combined repeated-dose/reproduction/developmental toxicity screening test (OECD TG 422) on the C_{14}-C_{24} alkaryl derivatives to address these endpoints. The C_{14}-C_{24} alkaryl derivatives is the lower molecular weight member, which is presumably more bioavailable. The submitter is proposing to bridge these data to the polypropylene derivatives. EPA considers this approach appropriate.

Ecological Effects (fish, invertebrates, and algae).

No data are available for ecological effects endpoints. The submitter proposed testing for C_{14}-C_{24} alkaryl derivatves for all acute endpoints and bridging of these data to the polypropylene derivatives. However, EPA recommends no acute or chronic aquatic toxicity testing because the chemicals have estimated log Kow values greater than 8 and negligible estimated water solubilities, and therefore no toxicity is expected.

Specific Comments on the Robust Summaries

The submitter used EPIWIN version 3.04 to run its physicochemical properties and environmental fate estimations on CAS numbers 115733-08-9 and 68081-77-6. The submitter needs to provide the exact SMILES notation used for each chemical.

Environmental Fate

Transport and distribution (Fugacity). The submitter needs to incorporate in the robust summary the values of the input parameters used in the model.

Health Effects

The summaries omitted the purity of the test material.

Followup Activity

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.